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Risø National Laboratory, DK-4000 Roskilde, Denmark
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DEPARTMENT OF ENERGY TECHNOLOGY
ANNUAL PROGRESS REPORT
1 January - 31 December 1985

edited by
B. Micheelsen and F. List

Abstract. The general development of the Department of Energy Technology at Risø during 1986 is presented, and the activities within the major subject fields are described in some detail. Lists of staff and publications are included.

INIS-Descriptors: COAL; COMPUTERIZED SIMULATION; ENVIRONMENTAL IMPACTS; FLUIDIZED-BED COMBUSTION; HEAT TRANSFER; NATURAL GAS; PETROLEUM; POWER GENERATION; REACTOR PHYSICS; REACTOR SAFETY; REACTOR SIMULATORS; RESEARCH PROGRAMS; RISOE NATIONAL LABORATORY.

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CONTENTS

1. DEVELOPMENT DURING 1985

1.1. The Department of Energy Technology

In the spring of 1985 the Danish Parliament decided that nuclear energy should be taken out of the Danish energy planning.

In the Department of Energy Technology the theoretical thermohydraulic projects within nuclear safety research, on loss of coolant codes and heat transfer correlations, were terminated during the year. The reactor physics section still maintains a nuclear effort on theoretical reactor physics, and this work includes commercial work on nuclear reactor simulators, studies for the Danish research reactor DR 3, and theoretical safety services for the handling of fissile material at the Risø laboratories. Furthermore, the activities at the Danish reactor DR 1 were trimmed down during the year to allow a reduction of the staff by 70%.

In the non-nuclear field the reactor physics section increased its efforts on the environmental and the process simulation models, and a computer allowing the introduction of artificial intelligence techniques in the work was acquired.

The Heat Transfer and Combustion Section put a major effort into fluid bed combustion, where experiments were made on a 300-kW fluid bed and a cold test facility, and where work on a 2-MW circulating fluid bed pilot plant began. Furthermore, this section started activities on fundamental combustion research with a doppler laser anemometer.

The reservoir group worked on a large 3-dimensional reservoir simulator, and expanded the research work into large-scale basin modelling in co-operation with Danish universities and institutes.

1.2. Reactor Physics

Although the name of the section is still Reactor Physics, this topic occupies only a fraction of its activity and much of its work is directed towards areas not connected with nuclear power. During the year it was decided to co-ordinate the two areas of work in the section more closely. One is development of computer models for environmental impacts from energy systems, and the other is aerosol physics. The latter topic has evolved from the work of calculating consequences of large nuclear reactor accidents, that is, core melt accidents. The work up till now in aerosol physics has mainly been in this area. However, it is expected that the knowledge and methods shall be used in environmental studies.

Because of a loss of qualified personnel some of the research which was foreseen within the area of reactor physics has not been carried out. The major projects have therefore been limited to the verification of methods. A considerable amount of work has gone into the assessment of alternative designs for new cores with low enrichment for the Danish research reactor DR 3. In addition to the above, a development project related to the measurements of power distribution in LWR's, carried out for Scandpower, Norway, was completed by the beginning of the year.

In process simulation the aim of the research is to develop tools to facilitate the simulation of dynamic processes in industrial plants. Software is being developed that will enable the use of a library of modules each representing a standard component of industrial plants (e.g. pump, heat exchanger) is being developed. The software, which will have two pre-compilers, shall connect these modules into a model of a whole plant. Also a study of the advantages of artificial intelligence techniques has been incorporated into the research. To do this, an advanced workstation was installed during the year.

Although process simulation is now considered a research area of general interest, the major commercial project here was within the nuclear power field, from which area the topic originally developed. This was an extention of the simulation model for the Barsebäck nuclear power station. The model is now used in operation training. It is expected that projects in the future will fall mainly outside the area of nuclear power.

The work in aerosol physics was contentrated on core melt accidents, and a project on activity and aerosol release was carried out partly in cooperation with research institutes in the Nordic countries (the AKTI project). In addition, the section has followed the German Demona project, carried out as a part of Projekt Nukleare Sicherheit in Germany.

The state of development of the program system ECCES which is intended to predict environmental impacts from energy production systems has not changed significantly during the year. The main effort has been put into refining the models, collecting data and testing. Minor experimental studies to verify models have been carried out as well. The knowledge about the reliability of the model system is now larger, and it is therefore reasonable to continue further development of new submodels. Thus, the next step will be to concentrate on forest systems.

1.3. Heat Transfer and Combustion

Coal combustion and implementation of measurement techniques for important combustion parameters have formed the main part of the work during the year.

The work within fluidized bed combustion has been concentrated on circulating fluidized bed combustion and experiments to study sulphur dioxide removal from flue gas by adding limestone to the combustion process. Desulphurization processes have been investigated by measurements performed in a 300-kW atmospheric bubbling fluidized bed and in an electrically

heated small scale fluidized bed. Flow phenomena in circulating fluidized beds have been studied in a cold test facility made of glass tubes.

A 2-MW circulating fluidized bed pilot plant has been designed and is now under construction in the experimental hall. The first test run in this facility is expected in early spring 1986. During the year several commercial flue gas measurements have been performed at Danish power plants and industry.

The establishment of a laboratory for research on basic combustion parameters was initiated. A 3-beam Ar-ion laser doppler anemometer to measure local velocities of gas and particles during combustion has been purchased.

The last work in the nuclear field, the joint Nordic safety projects on small-break, loss-of-coolant codes (SAK 3) and heat transfer correlations (SAK 5) was completed during the year.

In the theoretical field two projects on computer modelling of flow phenomena are being pursued. In the first a steady 3-dimensional turbulent gas/particle flow in a combustion chamber is modelled. The second studies transient two-phase oil/gas flow in a pipeline.

The temperature calibration laboratory has calibrated thermometers for both internal and external customers during the year. The amount of work has been at the same level as the previous year.

1.4. Reservoir Group

The development of a 3-dimensional, fully compositional double permeability, reservoir simulator is well under way. New mathematical and numerical methods have been developed in collaboration with the Technical University of Denmark. A black-oil

version of the simulator has been tested with good results.

A computer code for generating simulator input data has been developed. Further developments based on geostatical methods are anticipated.

Simulations for the GORM North Sea field have been performed with a black-oil simulator. One member of the group has been involved in simulations for the TYRA gas field using the volatile-oil simulator, ECLIPSE.

Work has continued on basin models, simulating burial and temperature history and maturation of sedimentory basins. A preliminary project supported by the Danish Ministry of Energy will be followed in 1986 by a large-scale basin modelling project involving a number of university institutes, the Geological Survey and Risø.

The group's participation in the Danish aquifer heat storage project has continued.

1.5. Danish Reactor DR 1

The reactor has been used mainly for training purposes. Approximately 40 students from various universities have carried out experiments at the reactor over periods varying from 2-8 days whilst 27 high school classes have carried out experiments at the reactor, each class for one day.

In order to be able to improve and continue the courses at the present level, allocations have been applied for, and funds were granted from the Thrige Foundation and the Tuborg Foundation. These allocations will be used for procurement of a computer to be used in connection with an instrumentation for gammaray spectroscopy.

2. ACTIVITIES OF THE DEPARTMENT

2.1. A Low-power Model for the Barsebäck Power Plant Simulator

During 1983-84 a full-power model for the Barsebäck power plant was developed at Risø and transfered to the simulator running on a VAX 750 computer under the SIMNON simulation system at Barsebäck. This project was presented in the previous progress report. The Barsebäck staff has been quite satisfied with the simulator and in the beginning of 1985 they ordered a special low-power model for the power range 0-10%. It was developed during the year and installed at Barsebäck in November.

The model is made up of 6 modules which are:

1. The reactor module which simulates the neutron kinetics and the hydraulic dynamics in the reactor vessel, including the recirculation loops.
2. The control rod routine which takes care of all control rod movements including simulation of operators rod movements.
3. The feedwater control system.
4. The pressure control system.
5. The flux monitoring routine which simulates 3 flux channels and limit controls giving automatic interaction in the process.
6. The residual heat removal system.

Some main features which illustrate the difference between the low-power and full-power model are:

- The neutron kinetics and hydraulic dynamics are changed so the model can work down to room temperature and low pressure (1.5 bar). It required determination of new polynomials for neutron cross sections and steam/water parameters, and several modifications in the program.

- The recirculation circuit is simplified using one pump loop instead of four.

- The model structure has been changed to avoid small time constants for state variables; this allows larger integration steps as some transient simualtions run over many hours real time.

- The turbine and the feedwater preheaters are not included, and the feedwater control routine uses the auxiliary control system all the time with water intake from a tank at room temperature.

- The steam pressure is controlled by the coarse controller or the steam blow-down controller, and the hydraulic steam valve arrangement is very much simplified.

- A new routine for simulation of flux signals from three measurement channels is included and used for simulation of reactor start up.

- A simple model of the residual heat removal system with two heat exchangers is included.

- The model can be used to calculate steady-state conditions for input specified power and steam pressure conditions, and afterwards to calculate transients.

2.2. Development of a Simulation Tool

A tool is being developed to facilitate dynamic simulation of process plants on a computer. The basic concept is to use a two-step modulator approach. In the first step a module is assembled using submodules from a library, and in the second the modules are assembled in a connecting system that represents a mathematical model of the whole plant in question.

An existing simulation system (DYSIM) is being used to solve the equations set up to model the plant. The tool consists of two precompilers for presenting the equations in such a way that DYSIM can solve them.

The plant is divided into its natural sections and each section is being modelled in a module. The modules are constructed by the first precompiler (DYS/PRE1) and the other (DYS/PRE2) is used to assemble the modules and connect them to DYSIM.

The first precompiler (DYS/PRE1) has been developed. A module is being constructed by assembling submodules from a library. A submodule represents a unit in the plant such as a heat exchanger or an evaporator.

A syntax was chosen to present the information in the library that is needed by DYS/PRE1. The library is loaded from a file and the submodules can be included in the user's program. The kind of plant that is to be simulated determines the library to be used.

The user's program is written in one or more files, each containing one or more modules. The program is a series of commands subjected to a chosen syntax. The commands are used to include submodules from the library and to make assembling of modules with DYS/PRE2 possible.

A feature of DYS/PRE1 is that inclusion of a unit in the user's

program is not restricted to be done as a submodule. If the submodule needed is not present in the library it is possible in the user's program to write a series of standard Fortran 77 statements describing the unit in question.

Furthermore it is possible interactively to correct some of the syntax errors found by DYS/PRE1. After loading the library from its file the user can choose to keep either the old or the new version of the file, and the choice is also given after each of the files with modules have been compiled and corrected. The choice is given only if a correction was made.

2.3. Development of a Gamma-physics Model and its Implementation in RECORD

A subroutine calculating the response of a gamma-sensitive device in a LWR fuel box has been developed for Scandpower, Norway, and implemented in Scandpower's reactor physics code RECORD.

The gamma emission from all nuclear reactions is calculated in 5 energy groups (0-1, 1-2, 2-3, 3-4, >4 MeV) and the resulting gamma fluxes are determined by means of RECORD's diffusion routine (modified to enable fixed-source treatment).

The heating of a "gamma-thermometer" can then be calculated from the gamma flux and the energy absorption cross sections of the materials in the thermometer, or the response of a gamma sensitive counter can be determined by means of a precalculated response-function.

The work was finished, when "reasonably looking" results were obtained, and further verification is being carried out by Scandpower.

2.4. Analysis of the Relationship between Measured and Calculated Detector Response for a BWR Reactor

In 3-dimensional coarse-mesh solutions for power reactors there is no access to the detailed local flux at the detector position. One has to deduce the detector flux from average values of various reactor physical parameters of the surrounding fuel assemblies.

Three different calculation methods have been analysed (Nonbøl,1985).

1. Power Method
2. Normalization Method
3. Modulation Method

The power method simply assigns the average power of the 4 neighbour assemblies to the detector response.

The normalization method weights equally the fission rate at the detector position obtained from 4 separate 2-dimensional single-assembly calculations.

Finally, the modulation method is made by multiplying the results from the normalization method with a function taking the overall power distribution into account. This function is calculated from the average power of the 9 nearest fuel assemblies applying bivariate interpolation.

All 3 methods are compared with a detailed fine mesh calculation, and finally tested against TIP-measurements on the Brunsbüttel reactor.

The conclusion from the analyses is that none of the methods seem to give correct results. The modulation method appears to be the best, but it fails for assemblies with control rods.

One way to improve the treatment of detector response could be

to represent the boundary conditions of each assembly in a better way. If the net current at each of the four boundaries of the assembly had been available from the coarse mesh calculation it would have been possible to calculate the pin power distribution inside the assembly analytically and thus also the detector response.

REFERENCE

NONBØL, E. (1985). Analysis of the Relationship between Measured Detector Response and Calculated Detector Response for BWR Reactors. RP-15-85.

2.5. Reactor Physics Analysis of a Proposal for a New Core Design for the Danish Research Reactor DR 3

The Danish Research Reactor DR 3 may have to convert its fuel from highly enriched uranium (HEU-93%) to low-enriched uranium (LEU20%). Converting to 20% LEU fuel and sustaining the thermal power level at 10 MW leads to a 15% reduction in the thermal neutron flux. This is caused by the increased amount of U^{235} necessary to compensate for the absorption in U^{238}.

The reduction in thermal flux is very unsatisfactory for the users of DR 3 and therefore a new core design called ring-core has been considered as a possible way to remedy this (Haack,1985). In this design 4 central fuel elements of the total 26 elements are replaced by 4 dummy elements containing heavy water. The uranium content of the remaining elements is increased by an amount corresponding to the removed uranium. The purpose of the design is to obtain an increased thermal flux in the center of the core and thus compensate for the flux reduction caused by conversion to low-enriched fuel.

The 3-dimensional calculation model DR3/SIM (NONBØL, 1985) has been applied to a reactor physics analysis of the proposal for a new core design.

In Fig. 1 the average, axial thermal flux of the 4 central fuel elements for the new design (LEU-10-RingCore) is compared with the corresponding flux for the old design (HEU-10). The increase of the flux is about 7%.

Figure 2 shows the thermal flux in the remaining 22 fuel elements where the ring-core flux is reduced with about 12% compared with the old design.

Finally Figs. 3, 4, 5, and 6 show a 3-dimensional, qualitative picture of the fast and thermal flux for the new design compared with the old design. They clearly show how the removal of the 4 central fuel elements causes a "hole" in the fast flux and a peak in the thermal flux.

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HAACK, K. (1985). Means of Preserving Irradiation Qualities after Conversion to Low Enriched Uranium Fuel. IAEA-SR-119/26. Seminar on Applied Research and Service Activities for Research Reactor Operations. Copenhagen 9-13 September 1985.

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International Meeting on Reduced Enrichment for Research and Test Reactors (RERTR). Petten 14-16 October 1985.

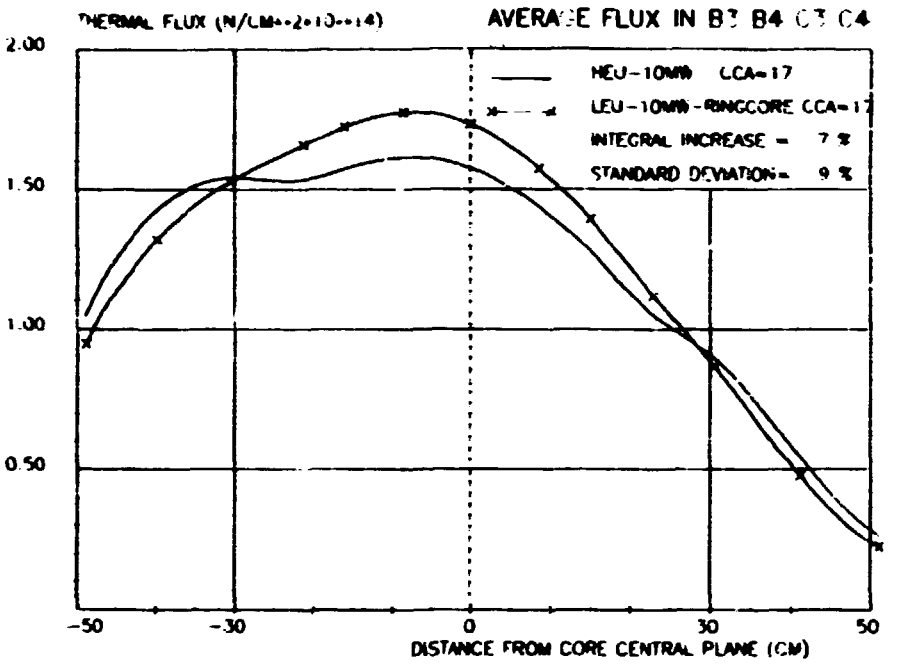

Fig. 1. Average axial thermal flux in the dummy elements.

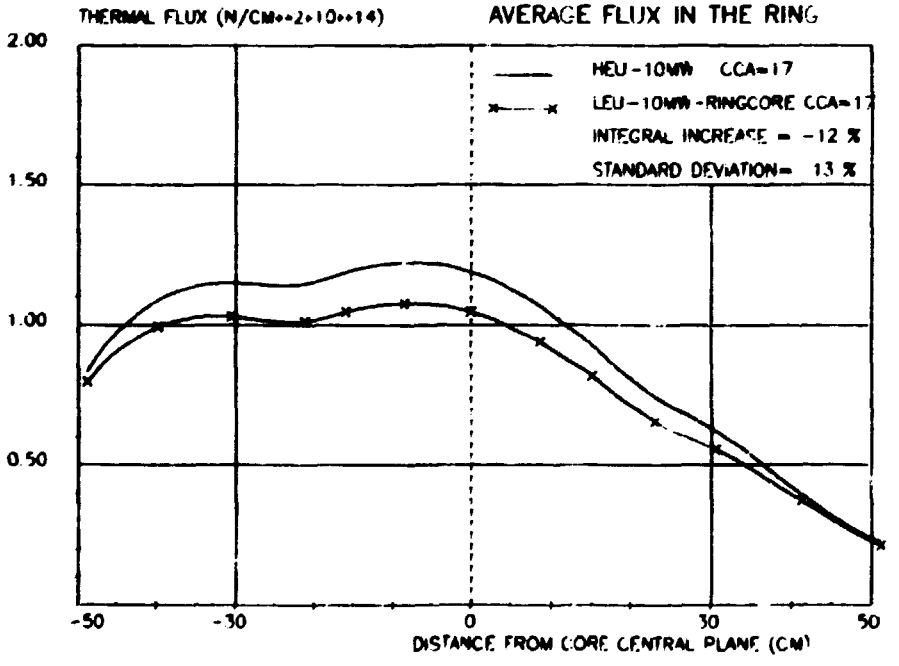

Fig. 2. Average axial thermal flux in the fuel elements.

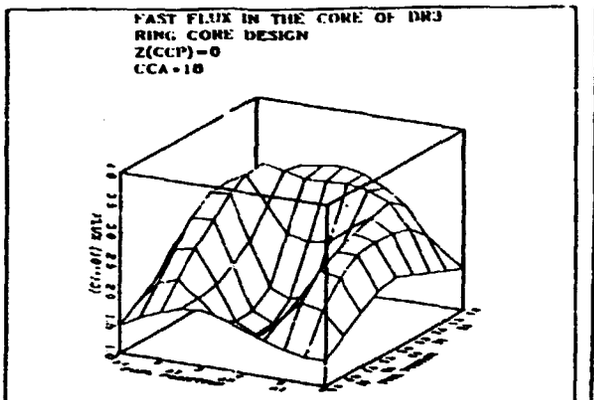

Fig.3. Ring-core design

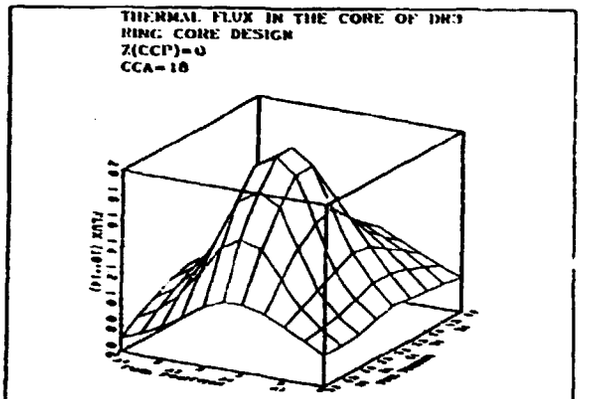

Fig.4. Ring-core design

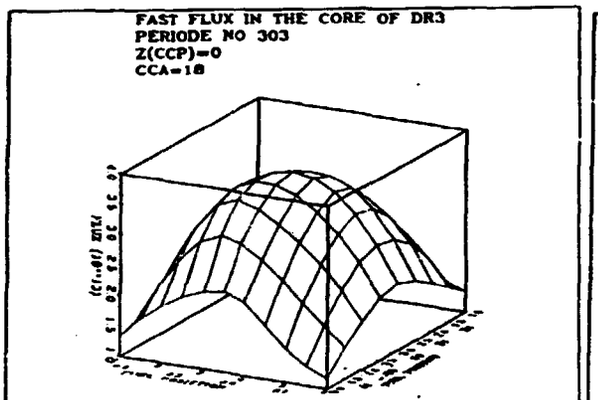

Fig.5. Normal(old) design

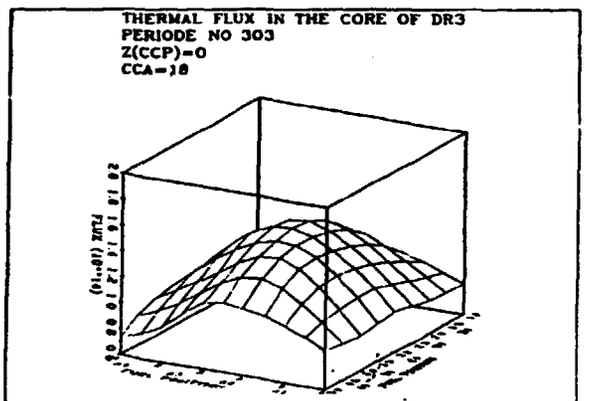

Fig.6. Normal(old) design

2.6. Aerosol Physics

In 1985 a Nordic 4-year collaborative project was initiated to study problems related to the release of radioactivity in the event of a nuclear reactor accident. The project is financed partly by the Nordic Liaison Committee for Atomic Energy (NKA), partly by the participating institutions themselves. One part of the project called AKTI concentrates on phenomena taking place inside the reactor building, and as aerosol physics plays an important part here, a working group was set up to cover this subject. The participants come from the Technical Research Centre of Finland, Studsvik Energy Technology, the Danish utility group ELSAM, and from the Department of Energy Technology.

The working group decided to start out by assessing the usefulnes of the so-called log-normal codes, i.e. codes using a log-normal size distribution for the aerosols, by comparing them to the NAUA code (BUNZ, 1983), which uses a groupwise representation of particle sizes and is considered one of the best, although time consuming, aerosol transport codes. The Danish part of the code comparison exercise was performed by ELSAM's and Risø's groups in collaboration and the log-normal code used was the HAARM-S code (HAGGBLOM, 1983). HAARM-S and NAUA were both run with 3 variants of a simplified "AB" accident sequence in a BWR. The aerosol behaviour under dry conditions in the containment was studied. In one of the variants 1600 kg of fission product aerosols were released during 169 minutes with a linearly increasing release rate followed by 600 kg of core/concrete aerosols during the next 60 minutes with a constant release rate.

Results from the codes were, among others, the particle size and the suspended, settled, and leaked masses as functions of time. Figure 7 shows how differently the codes predict the suspended mass in the atmosphere as a function of time. While the source is on (until about 3.8 hours) the log-normal code tends to overestimate the amount of material still suspended. After the source has been cut off and the aerosol left alone, however, the opposite happens. This means that if there is a leakage out of the containment from the start of the accident the log-normal codes will tend to predict high values for the integrated leaked mass which are too high because the leakage is proportional to the suspended mass. If, however, the leakage does not start to occur until a late point in the accident the log-normal approach may give results which are too low by more than an order of magnitude. Thus in both cases care must be taken in relying too much on the results produced by HAARM-S.

The great advantage of HAARM-S and other log-normal codes over a code like NAUA is the speed of computation. In the case studied the NAUA calculation took about 9 hours of CPU-time while HAARM needed less than a minute. This has led to an effort to

speed up NAUA. Various means to do this are being studied at the moment. For instance, a reduction of the number of size groups from 101 to 21 has reduced the computing time by a factor 9 for the test case in question. Whether this procedure is generally applicable, for instance also for wet cases, remains to be seen, however.

Further work in the aerosol working group comprises studies of factors other than the choice of size distribution which may be important to a proper description of aerosol behaviour and which are not yet modelled in the codes available. For instance such phenomena as resuspension, reevaporation, and nucleation processes are to be studied.

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BUNZ, H. et al., NAUA Mod4. A Code for Calculating Aerosol Behaviour in LWR Core Melt Accidents. Code Description and User's Manual. KfK-3554, August 1983.

HÄGGBLOM, H., HAARM-S, User's Manual, Version 1983. Studsvik/NR -83/298, September 1983.

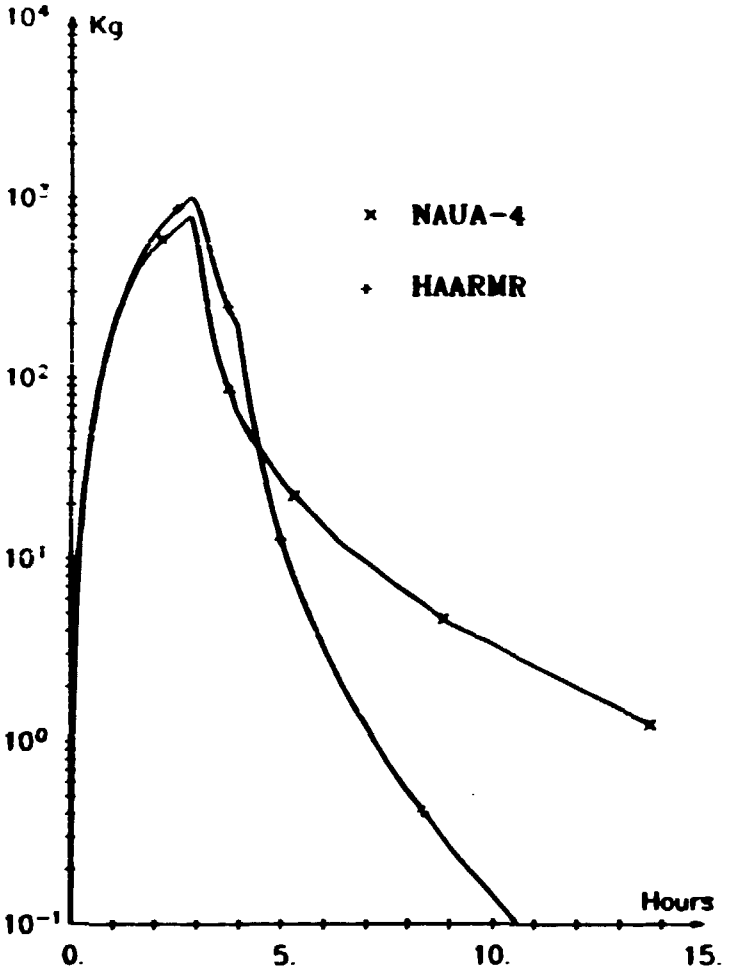


Fig. 7. Suspended mass in the containment atmosphere following the release of fission products from a molten reactor core and material from core/concrete interaction. Comparison of calculations with the codes NAUA-4 and HAARMR.

2.7. Model for the Environmental Impacts from Energy Production

The program system ECCES is designed to predict environmental impacts from a given energy production scenario in a given geographical area (PETERSEN, 1984).

Presently ECCES can follow transport and transformation of selected airborne pollutants (Cd, SO_2, NO_x) from sources via dispersion in the atmosphere and deposition on the ground to uptake in selected crops. Thus ECCES system contains submodels for dispersion and deposition, soil chemistry, and uptake of ions in crops. These three models are assembled in a single program, ECCES, where it is possible to run the three models independently or in common.

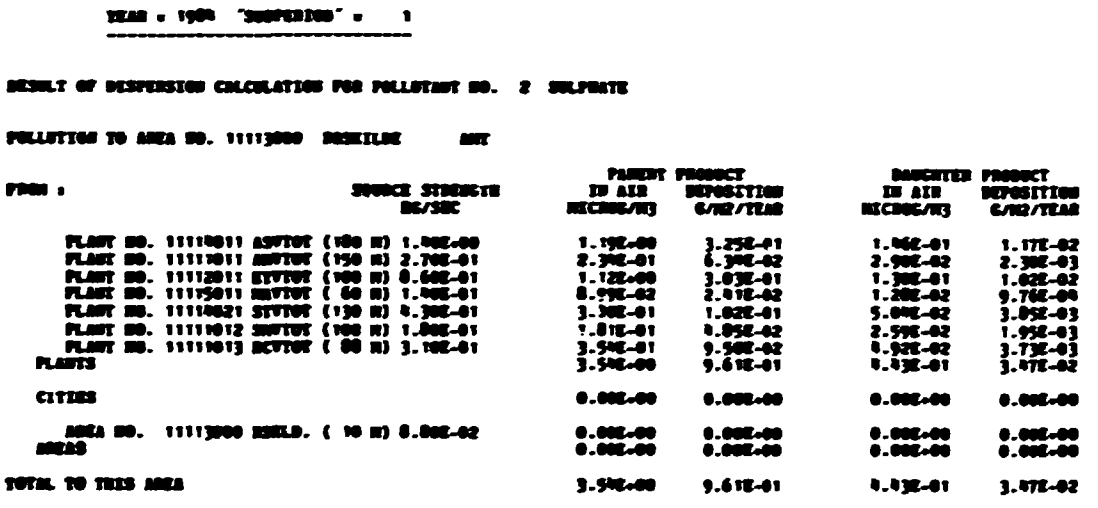
The dispersion model is able to calculate dispersion of pollutants from a number of sources to a number of recipients. The sources are the point sources: power plants and area sources: cities and counties (Danish: amt). The actual sources can be selected in a library of plants, cities, and areas. The sources are characterised by their coordinates in a cartesian coordinate system and by the source strength (kg/sec) for each pollutant at maximum energy production for each source. For power plants, moreover, the chimney height is given (HØJERUP, 1984).

The soil chemistry model starts where the dispersion model ends, namely with the deposition as input to the model. The soil chemistry model can be used in conjunction with the dispersion model or alone. If it is used alone it is possible to select one or more soil types from a soil type library. The soil type library contains data such as the number of layers, the water capacity for each layer, the ion exchange capacity for each layer, etc. Today 7 different typical Danish soil types have been defined. The soil chemistry model alone calculates chemical equilibrium in each soil layer (BRODERSEN, 1984).

The crop model is the third and last module in the simulation complex and this module demands at least that the soil chemistry model also be used. It is possible to simulate uptake of ions in different crops and again the actual crop data are selected through the input from a crop library. This library contains information about crops, such as biomass, water uptake, etc. for each month in the year. Ion uptake is proportional to the equilibrium concentrations of the ions in the soil water (MORTENSEN, 1984).

As an example of the capacity of the model a scenario with Roskilde county and seven power plants at Zealand (Asnæsværk, Amagerværk, Kyndbyværk, Masnedøværk, Stigsnæsværk, Svanemølleværk, and H.C. Ørsted plants) has been set up. Two different crops: winter cereals and grass are simulated in Roskilde county. This scenario is simulated first for 20 years with the power plants at full power and then further for 10 years with all power plants at zero power.

The results of the dispersion calculation for sulphur (SO_2 and SO_4^{--}) are shown in Fig. 8.



YEAR = 1988 "DISPERSION" = 1

RESULT OF DISPERSION CALCULATION FOR POLLUTANT NO. 2 SULPHATE

POLLUTION TO AREA NO. 11113000 ROSKILDE AMT

FROM :	SOURCE STRENGTH GR/SEC	PARENT PRODUCT IN AIR MICROGR/M3	PARENT PRODUCT DEPOSITION G/M2/YEAR	DAUGHTER PRODUCT IN AIR MICROGR/M3	DAUGHTER PRODUCT DEPOSITION G/M2/YEAR
PLANT NO. 11119011 ASVTOT (150 M)	1.00E+00	1.19E+00	3.25E-01	1.46E-01	1.17E-02
PLANT NO. 11117011 AMVTOT (150 M)	2.70E-01	2.39E-01	6.39E-02	2.90E-02	2.30E-03
PLANT NO. 11112011 KYVTOT (100 M)	8.60E-01	1.72E+00	3.03E-01	1.30E-01	1.02E-02
PLANT NO. 11115011 MAVTOT (60 M)	1.00E-01	8.99E-02	2.81E-02	1.20E-02	9.76E-04
PLANT NO. 11114021 STVTOT (130 M)	8.30E-01	3.30E-01	1.02E-01	5.04E-02	3.85E-03
PLANT NO. 11111012 SMVTOT (100 M)	1.00E-01	7.81E-01	8.85E-02	2.59E-02	1.95E-03
PLANT NO. 11111013 HCVTOT (80 M)	3.10E-01	3.54E-01	9.50E-02	4.92E-02	3.73E-03
PLANTS		3.54E+00	9.61E-01	4.43E-01	3.47E-02
CITIES		0.00E+00	0.00E+00	0.00E+00	0.00E+00
AREA NO. 11113000 ROSKILD. (10 M)	8.00E-02	0.00E+00	0.00E+00	0.00E+00	0.00E+00
AREAS		0.00E+00	0.00E+00	0.00E+00	0.00E+00
TOTAL TO THIS AREA		3.54E+00	9.61E-01	4.43E-01	3.47E-02

Fig. 8. Examples of printout from dispersion model. Parent product is SO_2, daughter product SO_4^{--}. (CHRISTENSEN, 1985).

An example of cadmium concentration in the harvest of winter cereals and grass in Roskilde county during the same 30-year period is shown in Fig. 9. A characteristic drop in the uptake when the power plants are shut down is seen.

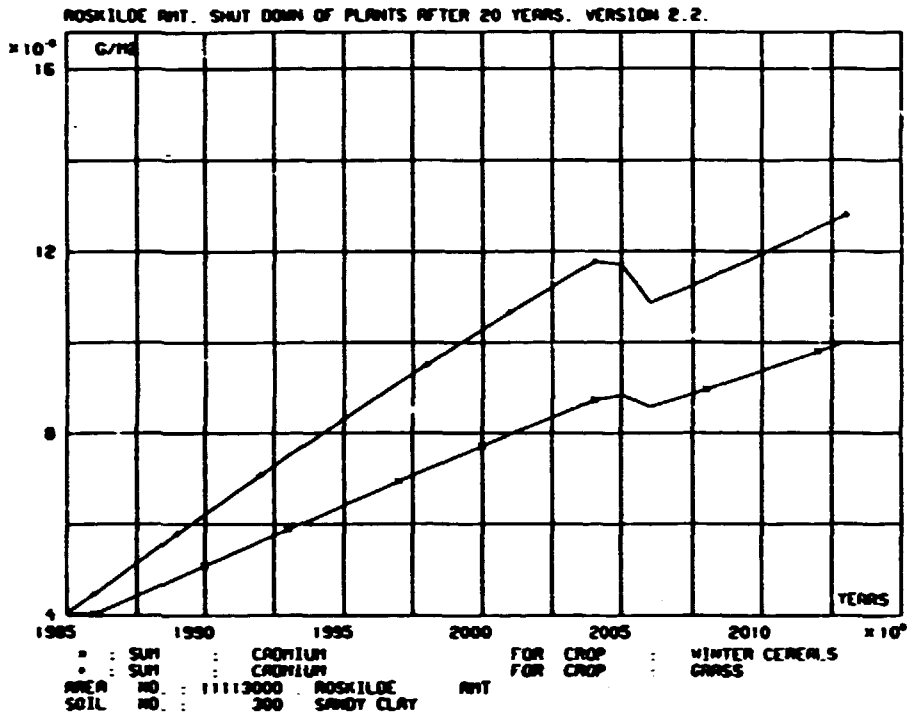


Fig. 9. Uptake of cadmium in the harvest of winter cereals and grass in Roskilde county during a 30-year period. (CHRISTENSEN, 1985).

The calculations shown are only meant to illustrate the present capabilities of the environmental program ECCES and in this stage of development are not intended to represent situations which can be encountered in nature.

The ECCES model is able to simulate soil chemistry experiments. Experiments with 5 g soil (dry weight) in 25 ml demineralised water continously washed out with 25 ml demineralised water (pH = 5.6) are shown in Fig. 10. Simulation of these experiments with different CECV (Variable cation exchange capacity) of 1, 4, and 9 meq/100 g and a constant CECP (Permanent cation exchange capacity) of 9 meq/100 g showed a high buffer effect of CECV. A constant pCO_2 = 0.002 atm (CO_2 partial pressure) is assumed. Other estimates of pCO_2 have given a high pH sensitivity. Thus determinations of CECV and pCO_2 are important for realistic calculations of soil acidification. A CECV of 9 meq/100 g seems to fit the experiment well.

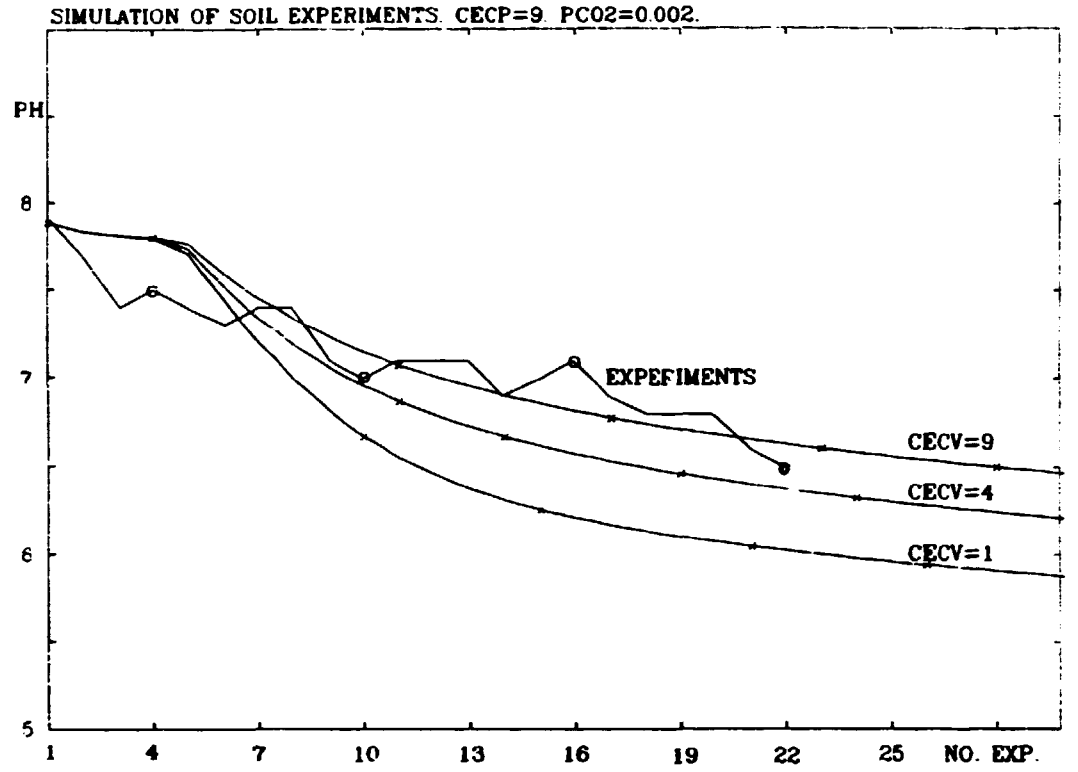


Fig. 10. Development of pH in soil experiment (O) and simulations with different CECV values.

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4.8. SAK-3: Assessment of Codes for Small-Break LOCA's.

The Nordic reactor safety research project SAK-3 aims at recommending one or more computer codes for analysis of Small-break LOCA's (of the Three Mile Island type).
The project, which has run over the period primo 1981 - fall 1985, is performed in cooperation with the Nordic institutes: Technical Research Centre of Finland, Studsvik Energiteknik AB, Sweden, and Institute for Energy Technology, Norway.
It was partly funded by the Nordic Liaison Committee for Atomic Energy.

The SAK-3 project consisted of theoretical and practical studies of a number of promising LOCA analysis computer codes: the two American codes TRAC-PF1 and RELAP5 and the Finnish small break code SMABRE. The practical study consisted of comparative calculations of 5 LOCA experiments:

1.	LOFT L3-6	2.5%	cold leg break, PWR, pumps running
2.	LOFT L3-5	2.5%	cold leg break, PWR, pumps stopped
3.	LOBI SD-SL-03	0.4%	cold leg break, PWR, LOBI mod. 1
4.	FIX-II-3031	48.0%	recirculation line break, BWR
5.	LOBI ISP-18	1.0%	cold leg break, PWR, LOBI mod.2

In 1985 "blind calculations" of the LOBI A2-81/ISP18 experiment were performed. "Blind" refers to the lack of knowledge about the experimental results until the calculations were finished. Some representative results of the calculations as compared to the experimental results are shown in Fig. 11.

A final report for the SAK-3 project was prepared. The findings obtained in the SAK-3 project, as expressed in the final report, are that the studied codes are able to predict

the over-all system behaviour (system pressure and temperature) rather well. Because of the nature of small breaks, the SMABRE code, although much more simplified and faster than the two large systems codes, performs as well as these. However, in cases where extensive phase separation occurs, as with stopped main calculation pumps, all of the codes fail to predict the steam/water distribution in the system properly. It seems that in order to remove this defect, so that the codes can be used for reliable small-break LOCA analysis, adequate models for stratified flow have to be implemented into the codes.

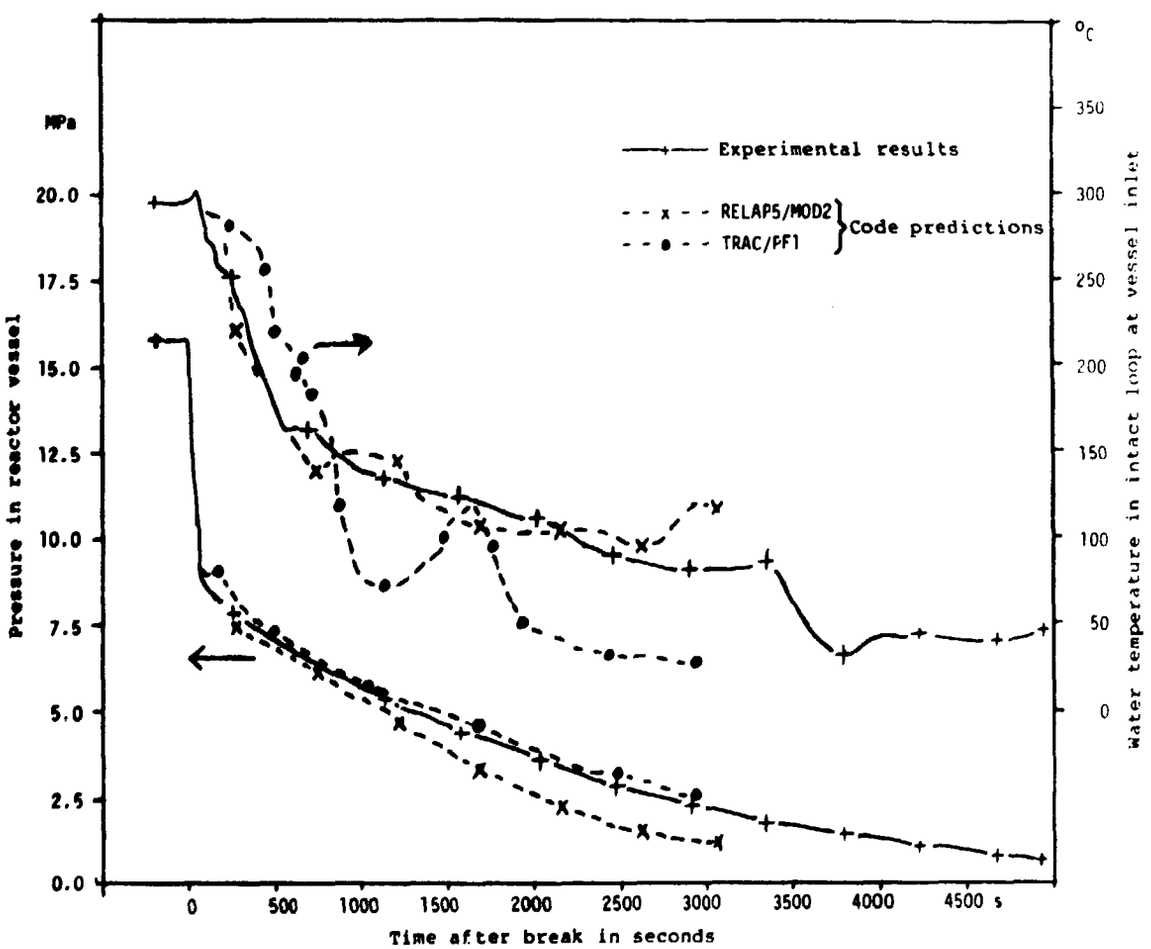

Fig. 11. Comparison of experimental results and code predictions for a small-break LOCA.

2.9. SAK-5, Heat Transfer Correlations

Like SAK-3, the SAK-5 project is a Nordic reactor safety project under the auspices of the NKA. The objective af SAK-5 is to provide a set of reliable heat transfer correlations, i.e. to contribute to the determination of the true wall temperature history of the fuel rod during a postulated accident.

The project has been closed down and a final report has been sent out (ABEL-LARSEN, 1985).

The conclusion from the work may be compiled in the following points:

1. The accuracy of heat transfer correlations in pre-CHF regions i.e. the nucleate boiling region and forced convective boiling region does not have to be very high for the purpose of calculating heat transfer during a loss-of-coolant accident (LOCA). The heat transfer in these regions is very efficiert and should not be a limiting factor for the fuel and the cladding during a LOCA.

2. With respect to critical heat flux (CHF) the examinations clearly indicate that Biasi and CISE-4 correlations do not predict the CHF conditions in large full-scale rod bundles. The correlations yield non-conservative results, and their use in computer programmes like TRAC and RELAP should be avoided. The Barnett correlation is valid only at 7 MPa pressure, so the Becker rod bundle CHF correlation is recommended within the following ranges: pressure 3.0 - 9.0 MPa, mass flux 400 - 3000 kg/m^2s and 0.5 - 3.0 MW/m^2. For mass fluxes between 100 and 400 kg/m^2s an interpolation of the Becker and the Griffith-Zuber correlations has to be made.

3. In the post-CHF region the transport phenomena should be considered in more detail to get more realistic

models. The post-CHF region should be treated as one region where the dividing point between transition boiling and film boiling is not the minimum film boiling temperature, but rather the point where the droplet can wet the surface or not. The surface can in fact be rewetted even if the minimum film boiling temperature has been passed, provided the momentum of the droplets perpendicular to the surface can prevail over the repulsive forces due to evaporation at the wall.

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2.10. The Temperature Calibration Laboratory

The Temperature Calibration Laboratory was accredited in 1978 by the Danish National Testing Board to carry out certified calibrations of temperature sensors in the -150°C to 1100°C range according to the International Practical Temperature Scale IPTS-68. The standard thermometers in the Laboratory are traceable to the National Physical Laboratory, England.

The number of calibrations for external customers has increased steadily during the years. In 1985 the Laboratory has performed 194 jobs for external customers and 4 for other Risø departments. In all 467 thermometers ranging from liquid-in-glass models to advanced digital types and 14 thermostats have been calibrated during the year. The calibrations have been made in the temperature region from -100°C to 1100°C which covers the main part of the range accredited.

2.11. Fundamental Combustion Research

There is a need for a more detailed knowledge about the fundamental combustion processes in order to make better computer models and thereby be able to construct better combustion equipment. By use of lasers it is possible to make non-perturbing measurements on flames, that can give information about the fundamental processes. In 1984 a laboratory was established for fundamental combustion research at the Department of Energy Technology.

The implementation of a Laser Doppler Anemometer is started. The LDA-equipment can make simultaneously measurements of velocities and turbulence in two dimensions.

Planning was begun of an experimental facility where the combustion of single coal particles can be studied.

A contact was made with Sandia National Laboratories in USA to collaborate on developing improved equipment for making particle size measurements in furnaces.

2.12. Coal Combustion in Circulating Fluidized Bed.

The development of a circulating fluidized bed boiler for industrial purposes, district heating, and power plants seems promising. The main reason for this is the possibility of achieving a high combustion efficiency accompanied by a large reduction of SO_2 and NO_x, which probably will meet the enviromental demands of the future.

The ongoing work is a part of a contract with the Ministry of Energy and it is performed in collaboration with a Danish boiler manufacturer. The main purpose of the work was to extend Danish know-how in this field. In 1985 work has been done in the following fields:

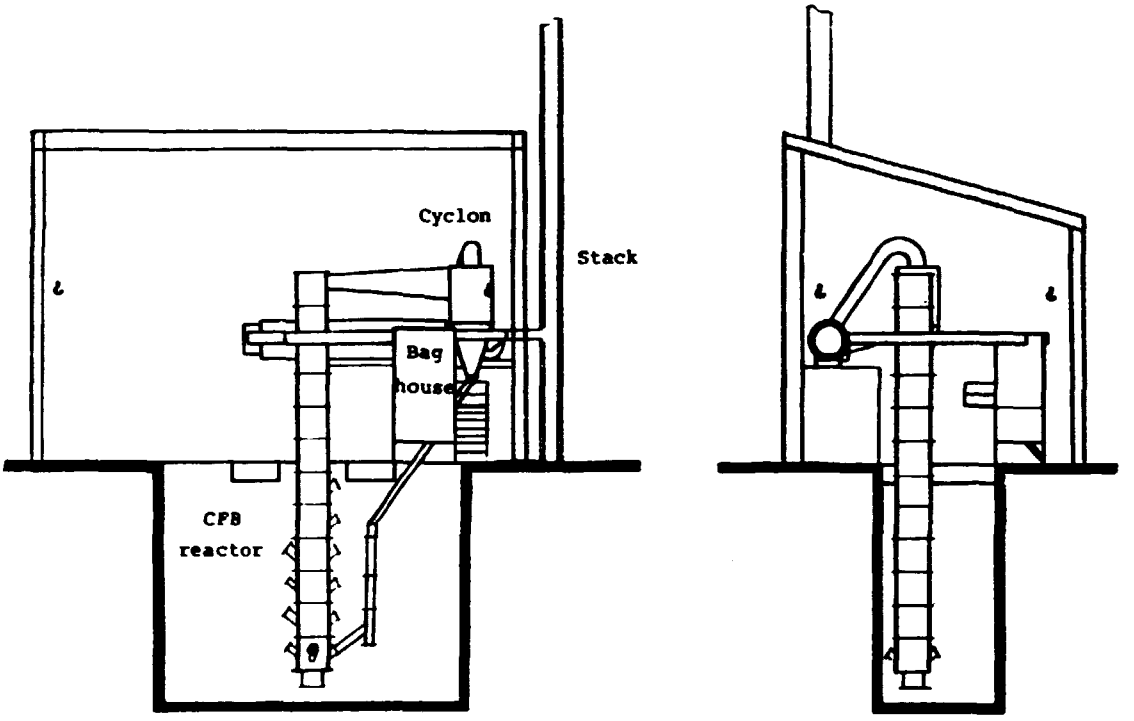

Fig.12. Main components of the 2 MW circulating fluidized bed (CFB) facility at Risø.

1. A cold running test facility, made in glass tubing, has been constructed, and basic experimental work has been done at this facility. The experimental data have given a lot of important knowledge about particle/gas flow in a circulating system.

2. In the last part of 1985 design and construction of a 2 MW circulating fluidized bed pilot plant has been started. The pilot plant (Fig. 12) is designed with a high grade of flexibility. This flexibility makes it possible to try different concepts without too much construction work. The first coal burning tests are expected to start in the first half of 1986.

3. In order to design the pilot plant some theoretical work has been done. The result is a performance program with simple models for combustion, heat transfer, and particle transport.

2.13. Sulphur Dioxide Removal from Flue Gases

Sulfur dioxide can be removed from flue gases by adding limestone. In fluidized bed combustion the limestone can be supplied directly into the combustion zone simultaneously with the fuel.

In a laboratory test facility 14 different commercially available qualities of limestone have been tested. The main part was of Danish origin, but for comparison also two from abroad have been tested. The four most promising types have been selected from the laboratory tests. These types have been tested in Risø's 300-kW atmospheric fluidized bed at real combustion conditions. Two types of limestone have been tested at the Danish Boiler Owners Association's test center in Vordingborg in a 1-MW fluidized bed. Finally, the best type of limestone will be tested in full scale in a 12-MW bed in a district heating station located in Skanderborg.

2.14. Computer Modelling of Steady Three-dimensional Turbulent Gas/Particle Flows.

Gas/particle flows are found in many industrial applications such as cyclone separators, pneumatic transport of powder and droplet combustion systems. The aim of the present work is to model the flow and combustion of coal particles with special reference to conventional furnaces for pulverized coal combustion.

Three main parts of the model can be identified. First, the turbulent flow of the gas and particles has to be determined. The second part models the devolatilization and combustion of volatiles and the combustion of the char residue. Finally, the thermal radiative heat flux between the gas, the particles and the walls of the furnace has to be modelled.

During the past year the development of the flow model has been initiated in co-operation with the Laboratory of Heating and Air-conditioning of the Technical University of Denmark. The two-phase model will be based on a single-phase steady 3-dimensional flow model being developed at the Technical University, and it will allow for unequal gas and particle velocities and turbulent particle diffusion.

There are two main approaches in modelling gas/particle flows: One is the use of the continuum or "two-fluid" model in which the particulate phase is regarded as a continuum in much the same way as the gaseous phase. This requires that the gas/particle flow is not too dilute. The equations of the two phases are coupled through the volume fraction of particles and through constitutive terms for mass, momentum and energy exchange. In the second approach, namely the trajectory model, the trajectories of an adequate number of particles are determined by integration of their equations of motion. The particle trajectories specify the sources of mass, momentum and energy to the gaseous phase, and these sources are used to correct the gas flow field. The new gas velocities change the particle trajectories resulting in new source terms and so on, until the solution has converged. The two approaches have both advantages and disadvantages, but preliminary investigations have indicated that a trajectory model is best suited for pulverized coal furnaces.

2.15. MULTWO: Compositional Computer Model for Transient Oil/Gas Two-phase Flow.

Oil/gas two-phase pipelines are of great technical and economic importance for offshore oil/gas fields, especially as connection lines between a central separation/pumping platform and a number of satellite fields sharing the platform. Computational tools in form of computer models may help solve the serious operational and safety problems associated with the use of two-phase pipelines.

With this background, in 1984 the first phase of the development of the MULTWO computer model was performed in cooperation with LICconsult Consulting Engineers Ltd. and the Institute for Chemical Engineering of the Technical University of Denmark.

The first development phase resulted in the basic framework of the computer code, allowing for a description of the oil/gas flow in pipelines by a fully integrated calculational scheme for time- and position-dependent compositions, volume fractions, velocities, pressure and temperature of the two phases (equal pressure and temperature for gas and oil).

In 1985 the calculational method has been fine-tuned, and new flow-pattern models (partly developed during the 1984-work) has been implemented, especially for stratified and annular flow.

Hypothetical time-dependent test cases have ensured that the models simulate the propagation of pressure waves and surface waves qualitatively correct. Quantitative tests have been performed by comparison with various available steady-state measurements, e.g. from the Friggs - Sct. Fergus line in the North Sea. These tests indicate that in stratified flow the pressure loss may be predicted with an accuracy comparable to that in single-phase flow. However, the prediction of liquid holdup (volume fraction) depends on the assumed roughness of the gas/liquid interface. At present, one can give only upper and lower limits for this roughness, whereas a physical/mathematical model for the interface roughness requires a separate development work, based on systematical series of relevant two-phase flow experimental data.

It is planned to test the MULTWO model further by comparative calculations of a longer series of experimental data available to the project, both from laboratory small-scale experiments and from full-scale pipelines.

The work has partly been funded by the Danish Ministry of Energy.

2.16 Compositional Reservoir Simulator

The black-oil reservoir simulator which has become traditional has served the oil industry well during the last decade. It has grown in reliability with the development of suitable numerical methods, and in sophistication with the growth of available computer power.

For describing natural depletion of oil reservoirs the black-oil simulator will still be the preferred simulation tool, but for some reservoir types and for a number of enhanced recovery methods the black-oil simulator is unsuitable. This, together with the access to increased computer power, has led to the development of a new generation of reservoir simulators, one of which is the compositional simulator.

The compositional simulator is characterized by a more detailed modelling of the hydrocarbon phase behaviour. It includes the simpler black-oil model and its extension, the volatile-oil model, but further covers the cases where hydrocarbon composition alters with time and position in space. The compositional simulator is consequently suitable for the simulation of gas recycling in gas reservoirs and for enhanced oil recovery methods such as CO_2-injection or N_2-injection and gives a more correct description of the gas injection in oil reservoirs.

The development of the compositional simulator, COSI, is well under way in a collaboration between Risø and the Laboratory for Energetics of the Technical University of Denmark.

COSI is a 3-dimensional, fully compositional simulator including double-permeability capability with the Danish fractured chalk reservoirs in mind.

COSI treats three or more phases with an arbitrary number of components. Phase equilibrium is defined by a general equation of state, including the standard equations by Redlich-Kwong and

Peng-Robinson as special cases. The more detailed data on phase behaviour needed for the compositional description are calculated on the basis of characterization analysis as performed by the Risø Chemical Department.

The double permeability description treats reservoir rock as two overlapping interconnected media, with mass exchange driven by pressure and concentration gradients. This feature is needed for a reasonable description of the fractured Danish chalk reservoirs.

New numerical methods have been developed to ensure absolute stability combined with low computing costs. Space integration is performed by means of a flexible integral finite-difference method, which avoids reference to any specific coordinate system. Consequently cartesian, cylindrical or irregular grids are handled with equal ease. The 9- and 7-point finite-difference schemes are contained as special cases. Faults and local grid refinement are easily handled. The time integration is implicit and ensures linear stability under all conditions. The resulting non-linear algebraic equations are solved very efficiently by a method reflecting the required degree of implicitness.

COSI has been tested with its black-oil option against other blackoil simulators on a number of test examples with good agreement. The fully compositional version of COSI should be available in early 1987.

Supplementary experimental and theoretical studies of the effect of fractures in connection with gas injection and water injection will be started in 1986.

2.17 Basin Models

The description of the history of sedimentary basins, including the modelling of source rock maturity and hydrocarbon generation, has become an important exploration tool.

Simulations of basin history - trying to predict source rock maturity and hydrocarbon generation, migration and accumulation - is of course of great interest in connection with the increased exploration activity in the Danish area. In this connection it may be of interest that mature source rock have been identified in Danish on-shore areas, but the amount of hydrocarbons generated are as yet unknown.

A one-dimensional computer model to simulate burial history, including sedimentation erosion and compaction, temperature history and maturation of sediments have now been developed in collaboration with the Geological Survey. The development so far has been the introduction of a model, suggested by Tissot and Espitalié (1975), describing the degradation of kerogen by a number of first-order reactions, based on the necessary activation energies.

The components of the kerogen are divided into seven classes. All but one of these may be converted to hydrocarbons and are classified according to the activation energy needed for their pyrolytic conversion. (Fig. 13). The activation energy represents the energy needed to rupture a given type of molecular bond, ranging from 10 to 80 kcal/mole.

The kerogen conversion is described by the six first-order reactions:

$$-\frac{dx_i}{dt} = k_i x_i \quad , i = 1, \ldots, 6.$$

where x_i is the amount of kerogen of class i and where the reaction rate is determined by the Arrhenius equation:

$$k_i = A_i e^{-E_i/KT}$$

where E_i is the activation energy, K the Bolzmann constant, T the temperature, and A_i depends on the class and origin of

the kerogen component. The temperature is a function of time including the effect of changing depth and changing temperature profile. This makes the estimates of the variations in heat flux and surface temperatures important.

Simulations for the Aars-1A well using the values for A_i and E_i, as well as the kerogen composition, as suggested by Tissot and Espitalié for terrestial kerogen, gave transformation ratios that seemed far too high when compared with other available data.

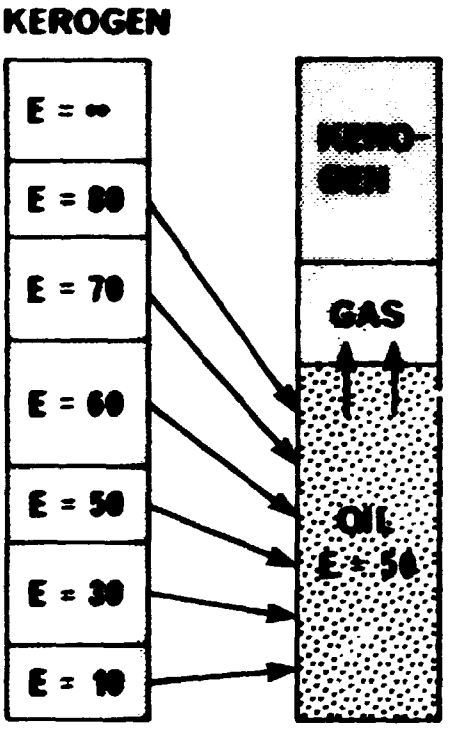

Fig. 13. Activation energies for kerogen conversion.

A parametric study shows the important effects of the assumed heat flux and surface temperature as well as the compaction. The results indicate nevertheless that the values for A_i and E_i as well as the kerogen composition, as published by Tissot and Espitalié, may have to be modified.

High-temperature laboratory experiments with relevant kerogens to determine A_i and E_i values are being considered.

A larger-scale basin modelling project involving the Geological Survey, a number of University institutes, and Risø will be started in 1986. The project will be supported by the Ministry for Energy, and will include the development of a 3-dimensional simulator to simulate hydrocarbon generation, migration and accumulation.

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